

POSTER PRESENTATION

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Exploiting solvent effects in drug design and optimization

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Upon ligand binding, solvent molecules around the binding pocket and the ligand become displaced or rearranged. These desolvation energies can be a significant portion of the total binding energy, and thus represent opportunities for ligand design. Computing desolvation energetics typically requires lengthy simulations, but this talk presents a fast and easy-to-use method (3D-RISM) which computes desolvation energies in minutes, without using explicit simulations. Application to ligand optimization is demonstrated using case studies.

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